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Determining Orientational Structure in Liquid Crystal Phases Using Resonant Polarized X-ray Diffraction

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Introduction: Resonant polarized x-ray diffraction (RPXRD) is a powerful technique to measure orientational periodicities in liquid crystals. A particular example of technological importance is the chiral smectic phases. In these phases, the rod-like molecules form layers within which the molecular long axes are tilted relative to the layer normal [See Fig. 1(a)]. The phases are distinguished only by the orientation of molecular tilt and no significant change in electron density, so ordinary x-ray diffraction does not provide structure information. By tuning the incident x-ray energy near the resonant edge of a sulfur atom in the core of the molecules, the scattering is sensitive to the orientation of the molecules. Resonant satellite peaks are observed at $Q_z/Q_0=L+M[(1/\nu+\varepsilon)]$ where L and M are integers and M=0,±1, or ±2 and ε corresponds to a longer periodicity on the order of optical wavelengths. Polarization and intensity analysis of the M=±1 and M=±2 provides a means to discriminate between models of the phases. Previously, RPXRD experiments confirmed a 4-layer periodicity in the SmC_{FI2}^* phase[1]. Polarization analysis supported a clock-like evolution of the molecular tilt within the 4-layer uniaxial repeat unit. Lorman proposed a model for SmC_{FI2}^* with a biaxial repeat unit shown in Fig. 1(b). This model is consistent with optical results[3]. With this biaxial repeat unit structure of SmC_{FI2}^*, an additional splitting (=ε/4) of the M=±1 peaks should occur with the intensity ratio of the split peaks related to the angle δ, describing the biaxiality of the repeat unit shown in Fig. 1(b).

Results: During the period covered by this Activity Report, the splitting of the resonant satellite peaks was observed. This was achieved by improving the resolution of the experiment by a factor of 3. Fig. 2 shows the peaks found in a study of a thiophene compound. The solid line indicates a simulation of the intensity for the structure shown in Fig. 1. The ratio of the peak intensities indicates that the angle δ is 15°, which is consistent with optical measurements. Furthermore, through polarization analysis of the first and second order resonant satellite peaks, we are able to demonstrate that the order of the molecular tilts in consecutive layers is that shown in Fig. 1. Other progressions, e.g. (c_1, c_3, c_2, c_4) are ruled out by the resonant scattering studies.

Future Directions: We have also used RPXRD to study the temperature evolution of a nm-sized incommensurate short helical pitch in the chiral smectic SmC_α^* phase. As well as continuing these studies, we will apply the technique to characterize the novel phases formed by banana-shaped molecules.

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References: [1] P. Mach *et al.*, Phys. Rev. E, **60**, 6793, (1999). [2] V. L. Lorman, Liq. Cryst. **20**, 267 (1996). [3] P. M. Johnson *et al.*, Phys. Rev. Lett. **84**, 4870, 4870 (2000). [4] A. Cady *et al.*, Phys. Rev. E **64** 050702(R) (2001).

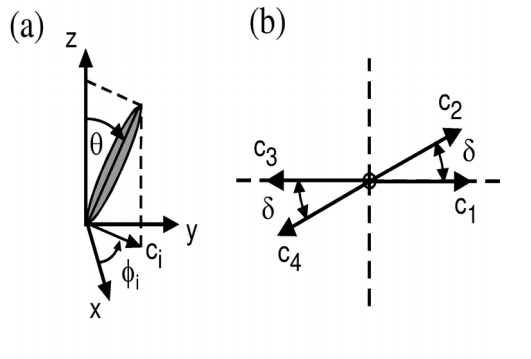

Figure 1. a) the azimuthal orientation of molecules In the *i*th layer. b) the biaxial model of the repeat unit

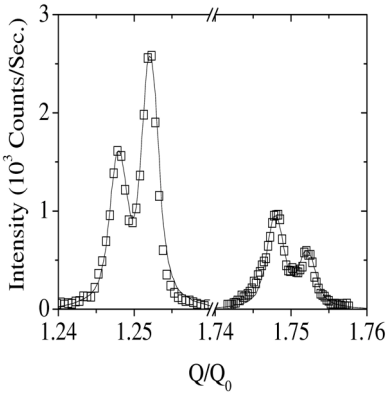

Figure 2. The first order satellite peaks (squares) and simulations (solid lines).